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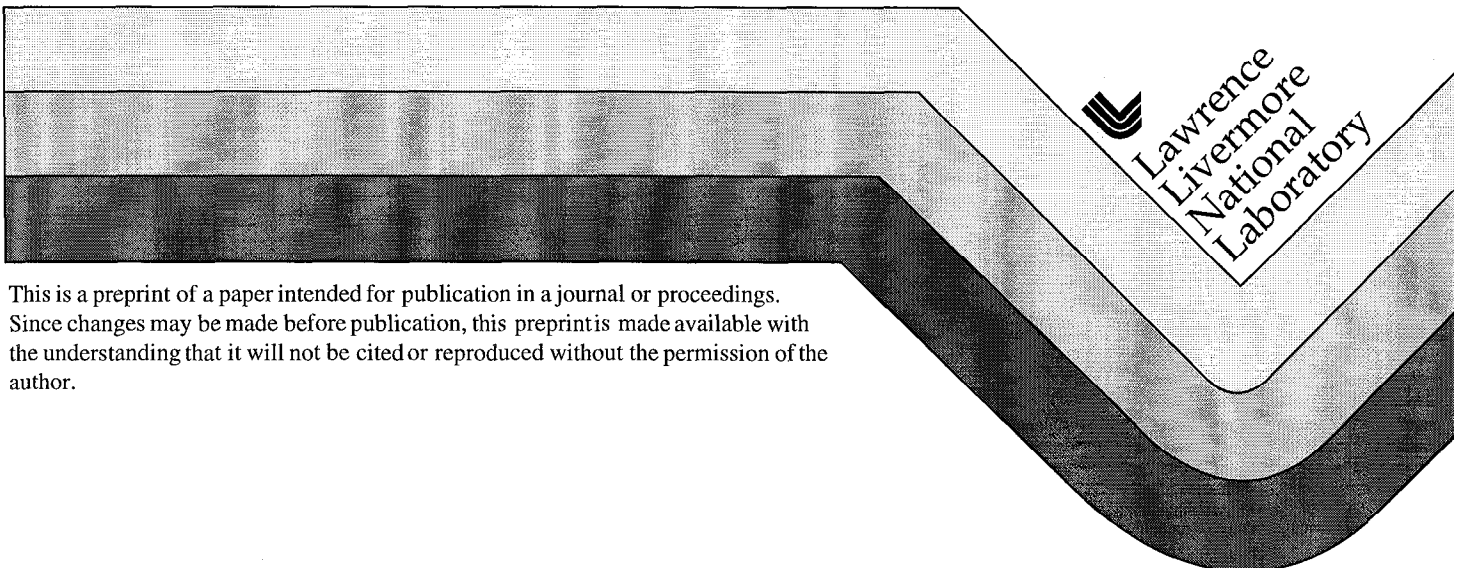
PREPRINT

Overview and Applications of the Monte Carlo Radiation Transport Tool Kit at LLNL

The Monte Carlo Radiation Transport Group
Presented by K. E. Sale

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Overview and Applications of the Monte Carlo Radiation Transport Tool Kit at LLNL

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ABSTRACT

Modern Monte Carlo radiation transport codes can be applied to model most applications of radiation, from optical to TeV photons, from thermal neutrons to heavy ions. Simulations can include any desired level of detail in three-dimensional geometries using the right level of detail in the reaction physics. The technology areas to which we have applied these codes include medical applications, defense, safety and security programs, nuclear safeguards and industrial and research system design and control. The main reason such applications are interesting is that by using these tools substantial savings of time and effort (i.e. money) can be realized. In addition it is possible to separate out and investigate computationally effects which can not be isolated and studied in experiments. In model calculations, just as in real life, one must take care in order to get the correct answer to the right question. Advancing computing technology allows extensions of Monte Carlo applications in two directions. First, as computers become more powerful more problems can be accurately modeled. Second, as computing power becomes cheaper Monte Carlo methods become accessible more widely. An overview of the set of Monte Carlo radiation transport tools in use at LLNL will be presented along with a few examples of applications and future directions.

1. Overview of Monte Carlo Calculations

The foremost reason for doing Monte Carlo radiation transport calculations is that they can save substantial amounts of time and effort. Monte Carlo calculations can be used to determine the feasibility of a radiation-based system. For example we have used such calculations to determine background event rates in a complex gamma ray detector in the presence of background neutrons. Another important application is to optimization of a system design, for example to maximize the yield of a spallation neutron source. In the early stages of a research and development project it may be important to determine which uncertainties are the most important. Numerical simulations can provide guidance in planning the basic science that needs to be done. Another way numerical simulations can help speed up the system development process is in providing simulated data (spectra, signals, backgrounds etc.) that can be used as inputs to the analysis algorithms. In this way data analysis algorithm development can proceed in parallel with hardware design and development rather than waiting for hardware construction to be completed.

The second important aspect of system simulation is the physical insight that can be gained. It is possible to do Monte Carlo experiments that simply can't ever be done in the lab, for instance separating out the signal contributions in a radiography system from direct and scattered radiation. Also ultimate limits of a system can be explored computationally by idealizing aspects of the system, e.g. simulating a perfect point source or a beam that is an exact delta function in time or energy. By exploring an ideal, wildly optimistic, unrealizable system it is sometimes possible to find fundamental difficulties with a proposed system and thus redirect efforts based on this information. The sorts of explorations that can be done using simulation can allow one to determine which specifications most strongly drive the system performance and which are relatively unimportant and not worth large R&D expenditures.

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The physics of a radiation transport problem usually resides in databases for photons and electrons and low energy neutrons and other hadrons (where low energy means up to 20, 30 or 150 MeV). When data bases don't exist physics models can be used. There are two main advantages of gathering the physics up into databases. The first is that the data are easily susceptible to inspection. A user can see exactly what is going into the calculation and confirm that the physics that is important is there. Also the data can be validated on its own without any transport. A second advantage is that data can be selected from different evaluations according to the user's taste, or if data is absent or a user has better data the data file can be edited. No change in the code is needed to see what difference using a different database makes. For high energy interactions the number of particles in the exit channel can be very large and such interaction are described by nuclear models. The data base approach becomes unwieldy because of the number of secondary particles and the correlations among them which would require excessive amounts of data storage. Another choice which will not be dealt with here is between continuous energy and energy group methods.

Another general consideration is the description of the world that is used. The geometry and materials of the system to be modeled must be specified. This is the area where there is the greatest divergence among the commonly used codes. Some codes permit an amazing array of geometrical surfaces, including almost any curve or surface seen in any analytic geometry text plus some very special surfaces. At the other extreme are codes which allow only surfaces defined by planes. The trade-off involved is essentially between computer time and human time. In each case it is up to the user to understand what is important in the problem at hand and choose the right level of complexity. In the same way the level of detail needs to be chosen. In some cases it may make sense to approximate a human as a water bucket, in others detailed information, say from a CAT scan, is needed to answer the question at hand. Again the trade-off is among accuracy, computing time and human effort.

The third general part of a Monte Carlo calculation is the question to be answered, e.g. energy deposition, reaction rates etc. The sorts of questions that can be addressed include, for example, performance of a detector in a high energy physics experiment with complex coincidence requirements or detailed dose maps in a radiation oncology treatment plan or dose rate at the fence line of an accelerator facility. Each of these questions requires a very different analysis phase of the Monte Carlo simulation.

2. Application Examples

2.1 Radiography with neutrons and photons.

In an assessment of airport security technology we created a model luggage item which contained several innocuous and a few threatening items. Figure 1 shows computed photon and neutron radiographs. These two images illustrate the relative strengths and weaknesses of the two radiography modes. These images also demonstrate the level of geometric detail that can be included if needed to simulate the real world as accurately as necessarily.

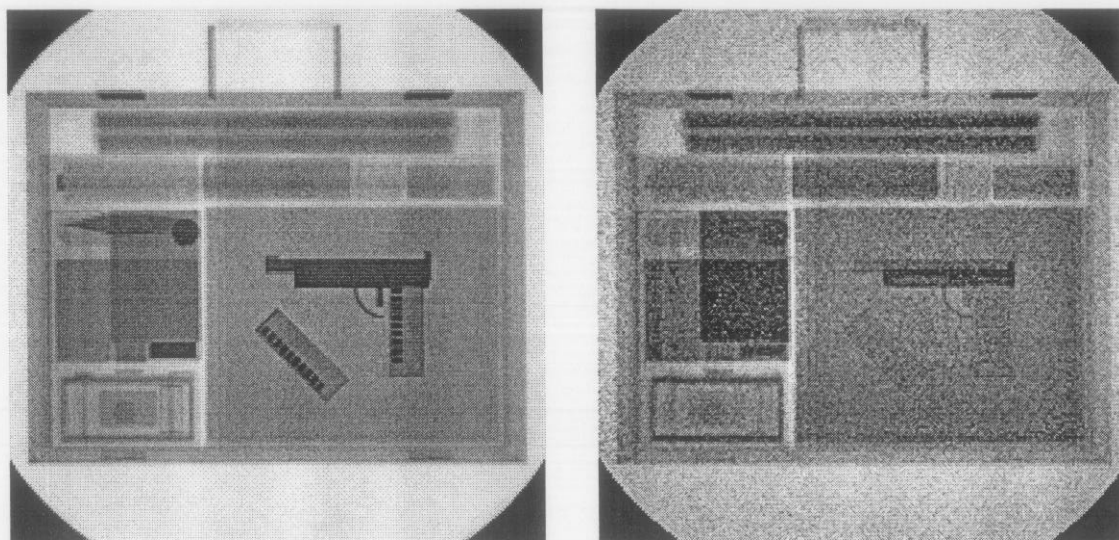


Figure 1. Photon (left) and neutron (right) radiographs. These images are courtesy of J. M. Hall, LLNL.

In the design of neutron radiography systems for luggage inspection the main parameter available for optimization is the energy (or energies) of the neutrons. Figure 2 shows a set of computed shadowgraphs. The upper row of images is from 453 keV neutrons and lower is from 638 keV neutrons. The calculated images are on the left side of the figure. The images on the right side show the contribution to the image from neutrons that have scattered at least once. The center images are the difference between the full and scattered-only images and correspond to neutrons that were unscattered and are described by Beer's law ($e^{-\mu x}$). This figure demonstrates a couple of important capabilities of numerical simulations. First, the scattered and direct contributions to the image could not be disentangled in a real system, in the simulation they can be. Secondly, the basic feasibility of the concept is addressed and the effect of varying the energy of the neutron beam is apparent. Thirdly, analysis algorithms (e.g. subtracting images made using different beam energies) can be explored and tested before hardware is even designed. In fact using such images a very thorough assessment of the false negative and false alarm rates of the proposed system can be quite reliably estimated.

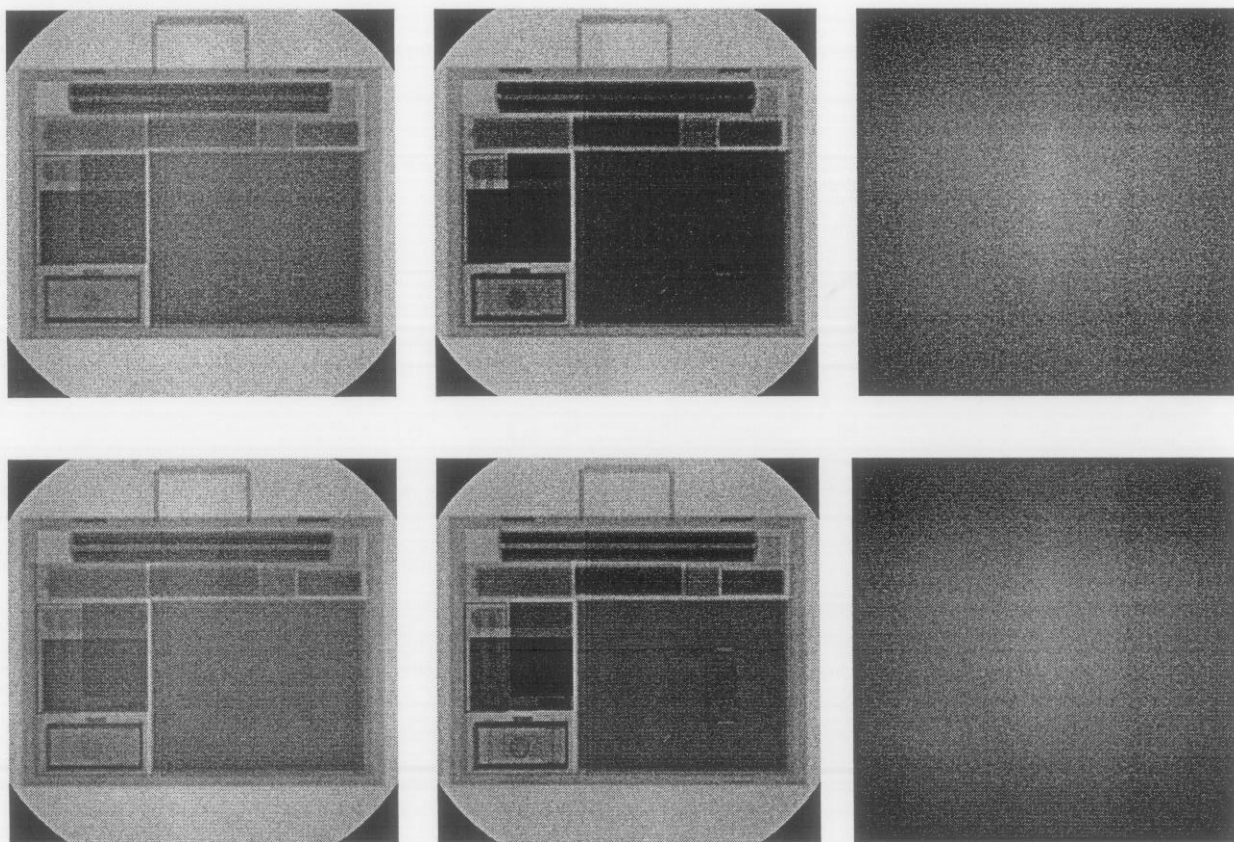


Figure 2. Neutron radiographs.

Computed neutron radiograph images of a suitcase containing among other items a loaded gun with a spare ammo clip, a camera, books, sheet and block high explosives and cotton and wool items with the approximate density of clothing. The top row of images is from 453 keV neutrons and the bottom row from 638 keV. The images on the left are full transport images while those on the right are from neutrons that have been scattered. The center images are the total minus scattered. These images are used courtesy of J. M. Hall, LLNL.

2.1 Radiation Oncology Treatment Planning.

Another area of application we are developing is medical treatment planning. The PEREGRINE system uses detailed models of photon teletherapy sources and beam modifiers to calculate accurate high-resolution dose maps which a radiation oncologist can use to evaluate the quality of a treatment plan. Figure 3 shows a schematic representation of the PEREGRINE model of the world. The substantial difference between the dose predictions of the conventional treatment planning tools and the PEREGRINE system are apparent in Figure 4.

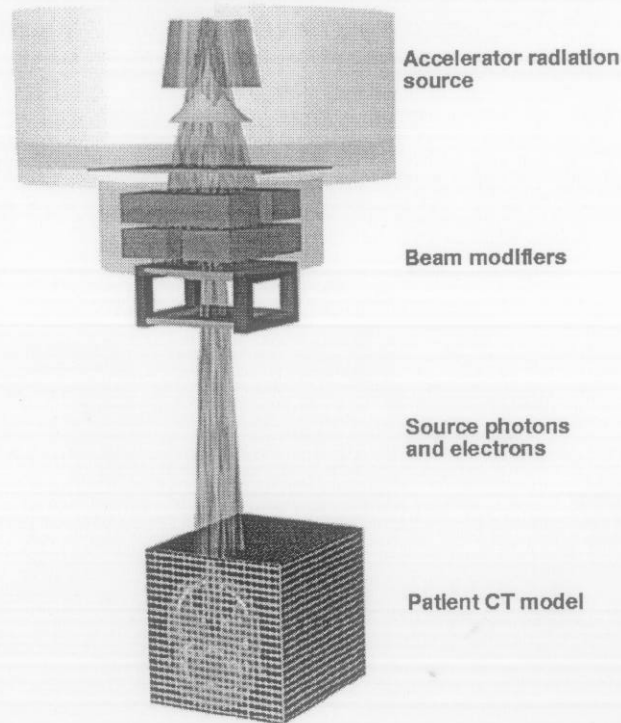


Figure 3. Schematic representation of a PEREGRINE calculation. The model includes a detailed source model tailored to a specific machine, moveable collimation slits and patient-specific beam modifiers and a high-resolution model of the patient derived from CAT scan data.

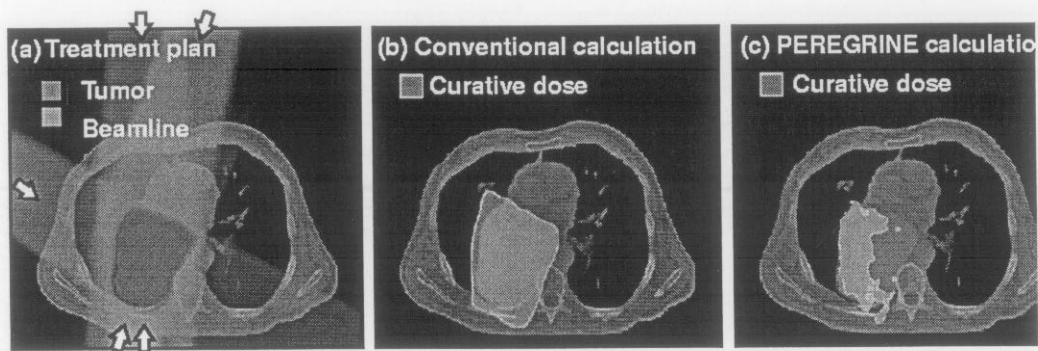


Figure 4. This lung cancer case highlights the importance of accurate dose calculations for providing correct dose coverage of the tumor and sensitive surrounding lung tissue. While conventional dose calculations show that the prescribed dose level covers the entire tumor (center panel), PEREGRINE calculations (right panel) suggest that for this treatment, the prescribed dose does not cover the entire tumor. PEREGRINE Monte Carlo calculations accurately account for photon and electron transport and in tissues of widely different densities and atomic compositions.

2.3 Accelerator Driven Transmutation of Waste.

An example of an application using several tools together is a calculation of the nuclide inventory history in an accelerator driven reactor waste transmutation system. This system is described by a set of coupled ordinary differential equations (ODEs) with coefficients that depend on the neutron flux spectrum. The neutron flux drives transmutation and fission which changes the material compositions which in turn change the neutron flux. To solve this problem we used an off-the-shelf ODE solver, which takes the coefficients of the ODEs as a function that it calls every time it needs a new set of values. The coefficient function took the present material composition and wrote an input file for the Monte Carlo Code (in this case TART) executed the code and read the flux spectra back in. This method is certainly not the most efficient one available in terms of computer time but since the pieces connected together so easily it was very efficient in terms of person-hours of effort. An example of a inventory history is shown in Figure 5.

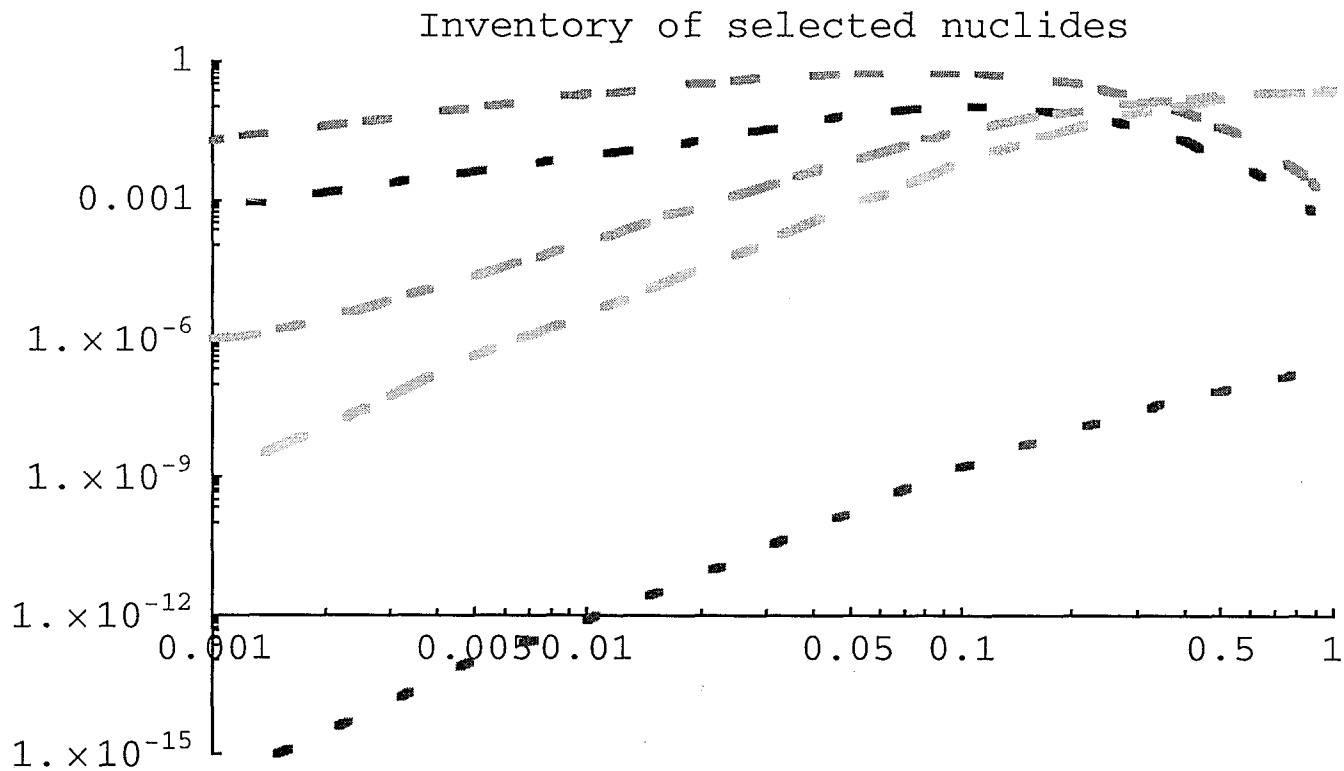


Figure 5. Inventory history for several nuclides in an accelerator driven waste transmutation scheme.

3. Present Status and Future Plans

We have three main radiation transport codes that the group is responsible for. COG is a coupled neutron-photon-electron database driven code with an extremely versatile geometry package. TART is a very robust coupled neutron-photon code with a simpler geometry package, which uses multigroup cross sections. TART features extensive debug tools for the users input and runs extremely quickly. There is already a well-developed interactive input preparation application for TART. PEREGRINE is a radiation treatment planning tool for photon teletherapy which is designed to interface with existing CAT scan systems to derive a model of the patient on a rectangular mesh. The expertise developed during the evolution and application of these codes has already begun to be captured in the Monte Carlo Tool Kit (MCTK) as general-purpose modules are extracted for use in other applications. Examples of such modules are data and input display and checkers and converters among various geometry description methods (e.g. converters for CAD file formats or hydrodynamic mesh routines). We also have gathered up robust, encapsulated routines to handle such tasks as thermal neutron scattering, photon

coherent and incoherent scattering and routines to handle multiband self-shielding for multigroup cross sections. In the near future modules for nuclear collisions at high energy (a few hundred MeV up to about one hundred GeV) will be developed and validated. Eventually we will be able to handle the entire particle zoo passing through material including the effects of electric and magnetic fields. Another area of major importance is the arena of user interfaces. A set of user-friendly GUI interface applications is being developed. Figure 5 contains a couple of screen shots of the new interface. All of our future development efforts will be undertaken with an eye toward filling the MCTK and building up a robust validated one-stop Monte Carlo shop.

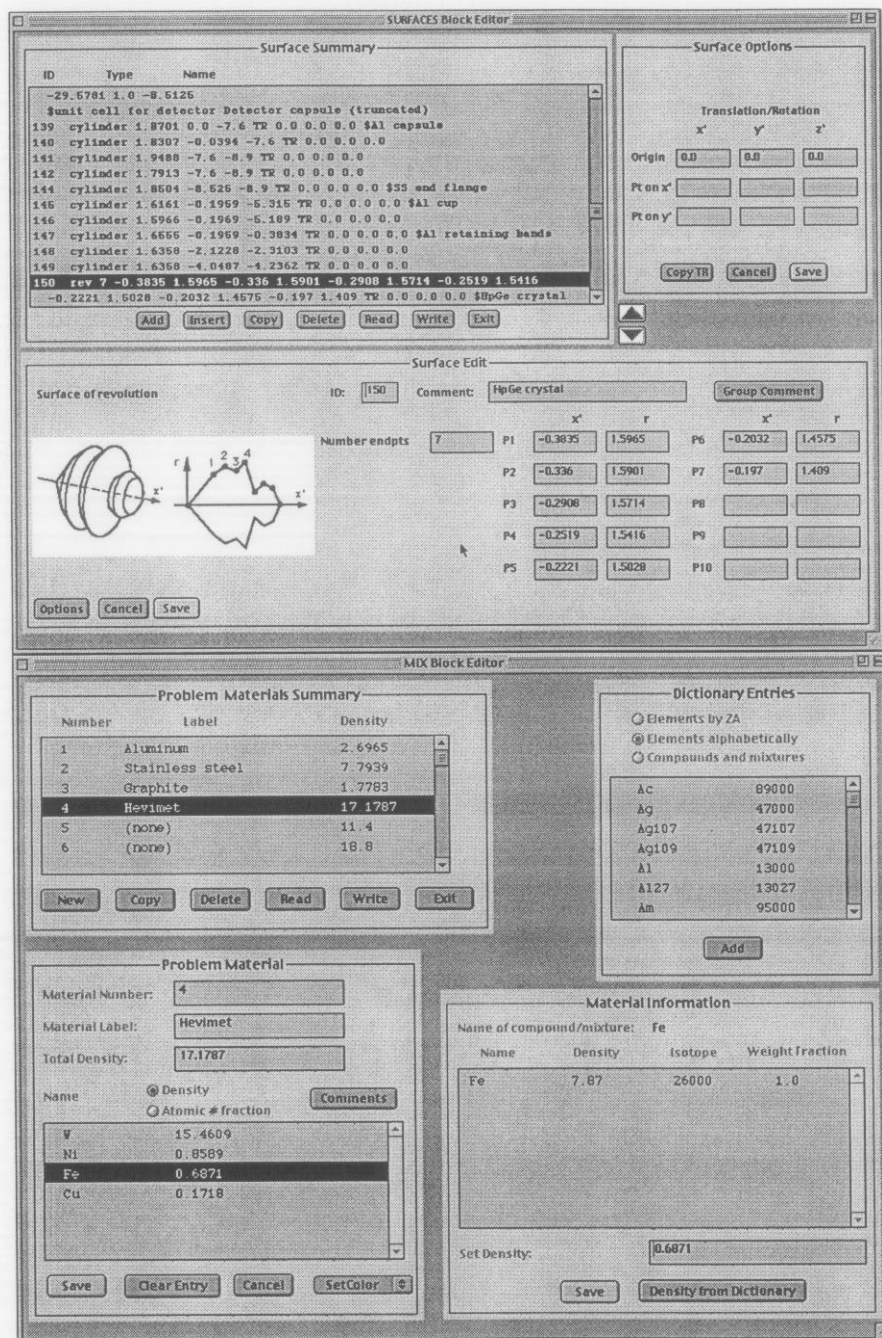


Figure 5. Example of the graphical interface being developed for generating input files. These images are courtesy of Susan Post, LLNL.

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